KIVA-4: An Unstructured Version of KIVA-3V

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KIVA is a name given to a series of multidimensional codes designed at Los Alamos National Laboratory to simulate internal combustion engines. KIVA was capable of computing transient compressible flow dynamics with fuel sprays and combustion in relatively simple two- and three-dimensional (2- and 3-D) geometries [1, 2]. KIVA-II [3] made much of the temporal differencing in KIVA implicit. While advection remained explicit with a subcycled time step, advection was made more accurate with an improved upwinding scheme. A k - ε turbulence model was also incorporated. KIVA-3 [4] added the capability of using a block-structured mesh where multiple blocks of cells could be patched together to construct a mesh. Software to generate block-structured meshes and post-processing visualization tools were included with the KIVA-3 package. The code was enhanced by a procedure (snapping) used to remove or add layers of cells during piston movement. KIVA-3V [5] added vertical or canted valves and a particle-based liquid wall film model.

KIVA-4 is the next generation of KIVA codes [6, 7] produced under the sponsorship of the DOE's Office of Freedom Car and Vehicle Technologies. While KIVA-4 maintains the full generality of KIVA-3V, it adds the capability of computing with unstructured grids. Unstructured grids, which include structured grids, are a more general class of grids. The unstructured grids can be composed of a variety of elements including hexahedra, prisms, pyramids, and tetrahedra. Unstructured grids can be generated more easily than structured grids for complex engine geometries. KIVA-4 also features a multicomponent fuel evaporation algorithm [8], where an injected liquid fuel can be composed of many types of fuels. In designing KIVA-4, an emphasis was placed on keeping the code comparable in computational efficiency to KIVA-3V. This entailed foregoing more expensive advection schemes. Current efforts are focused on completing the parallelization of KIVA-4 so it can run on multiple processors simultaneously.

Figure 1 (a) and (b) are a comparison of a 3-D engine computation with valves and injected fuel spray. The figures show color contours of fuel concentrations performed on a

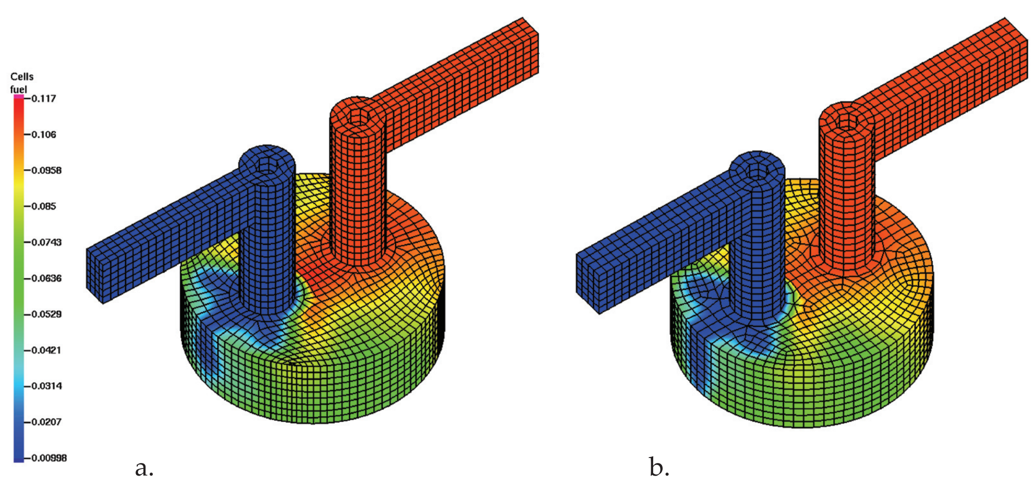

Fig. 1. ***The figures show a comparison of a 3-D engine computation with valves and injected fuel spray. They show color contours of fuel concentrations performed on a structured grid with KIVA-3V (a) and an equivalent unstructured grid with KIVA-4 (b). Despite differences in the grid and numerical schemes, both plots show similar distributions of fuel.***

structured grid with KIVA-3V (a) and an equivalent unstructured grid with KIVA-4 (b). Despite differences in the grid and numerical schemes, both plots show similar distributions of fuel.

Figure 2 shows the performance of a parallel version of KIVA-4 in a cylinder with 53,760 cells. The horizontal axis plots the number of processors. The red line shows the time required to complete 100 cycles. The green line shows the computational speed-up. The computational speed-up is the time required to complete the simulation with one processor divided by the time required to complete the simulation with multiple processors. One notices a puzzling trend in Fig. 2 when the number of processors exceeds 16. At this point, the amount of time spent communicating information between processors starts to offset the benefits of distributing the computational work to processors. In a larger grid, one would continue to realize improving efficiency gains with larger number of processors before encountering this communication penalty.

Our eventual goal is to have KIVA-4 adopted by industry and academia and used as a modeling tool to improve fuel efficiency and reduce fuel emissions in engines. A beta-version of KIVA-4 has been distributed to universities and industries to initiate collaborations and improve KIVA-4 with feedback we receive.

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[1] A.A. Amsden, et al., "KIVA: A Computer Program for Two- and Three-Dimensional Fluid Flows with Chemical Reactions and Fuel Sprays," Los Alamos National Laboratory report LA-10245-MS (Aug. 1985).
[2] A.A. Amsden, et al., "Improvements and Extensions to the KIVA Computer Program," Los Alamos National Laboratory report LA-10534-MS (Aug. 1985).
[3] A.A. Amsden, et al., "KIVA-II: A Computer Program for Chemically Reactive Flows with Sprays," Los Alamos National Laboratory report LA-11560-MS (Feb. 1989).
[4] A.A. Amsden, "KIVA-3: A KIVA Program with Block-Structured Mesh for Complex Geometries," Los Alamos National Laboratory report LA-12503-MS (Dec. 1992).
[5] A.A. Amsden, "KIVA-3V: A Block-Structured KIVA Program for Engines with Vertical or Canted Valves," Los Alamos National Laboratory report LA-13313-MS (May 1997).
[6] D.J. Torres, "KIVA-4: Validation, Rezoning, and Remapping," in *15th International Multidimensional Engine Modeling User's Group Meeting,* Detroit, April 2005.
[7] D.J. Torres and P.J. O'Rourke, "KIVA-4," in *14th International Multidimensional Engine Modeling User's Group Meeting*, Detroit, March 2004.
[8] D.J. Torres, et al., "Efficient Multicomponent Fuel Algorithm," *Combustion Theory and Modeling* **7**, 67–86 (2003).

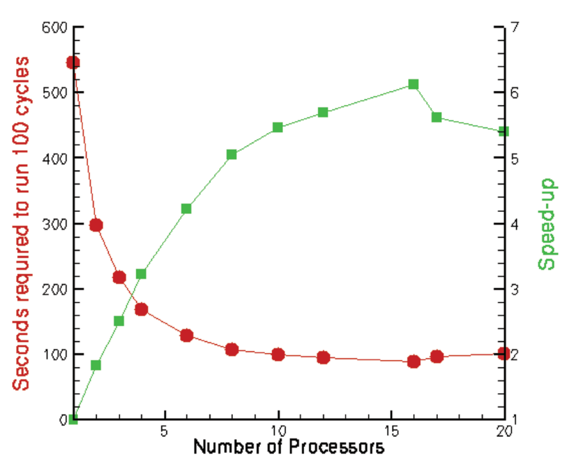

Fig. 2.
The performance of a parallel version of KIVA-4 in a cylinder with 53,760 cells. The horizontal axis plots the number of processors. The red line shows the time required to complete 100 cycles. The green line shows the computational speed-up.